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ELECTROMIGRATION AND THEROMOMIGRATION IN METALS.(U)
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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

electromigration	local field	electron-drag force
electrotransport	driving forces	electrostatic screening
thermomigration	microscopic field	Boltzmann equation
thermotransport	impurity scattering	Liouville equation
electron transport	electron-wind force	linear response theory

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The object of this research was to investigate theoretically the driving force for electromigration and thermomigration in metals.

The driving force for electromigration was shown to be equal to the local electric field accompanying electron transport. The force was determined from the linear response expression of Kumar and Sorbello using both the Green's function formalism and the Kohn-Luttinger formalism. Corrections to previous force expressions were derived.

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19. Key Words - continued

grain boundaries
residual resistivity
electron relaxation time
electron mean-free-path
electrical conductivity
electron charge density
Matthiessen's rule
Fermi surface
phase shifts
de Haas-van Alphen effect
dilute alloys
liquid metals
electron structure
dielectric response
phase shifts
distorted-wave Born approximation
memory function
force-force correlation function
ultrasonic attenuation
Dingle temperature
diffusion
heat of transport
effective valence
phonon scattering
electron-phonon interaction
electron-impurity interaction
screening breakdown
Green's function
electron self-energy
vertex corrections
Feynman-Hellmann theorem
pseudopotentials
lattice distortion
fast diffusion
Häffner effect
isotope effect
oscillator strengths
inversion layer
two-dimensional electron gas
MOSFET devices
activated complex

20. Abstract - continued

The effects of atomic configuration on electromigration was investigated within a pseudoatom picture. Application was made to lattice distortion, fast-diffusers, grain boundaries and isotope effects. Calculations were made of the driving force in liquid-metal alloys and were found to be in agreement with experiment. The Kohn-Luttinger formalism was applied to electromigration in an inversion layer.

The electron-impurity scattering responsible for electromigration was examined. Phase shifts were calculated and related to alloying properties. Agreement with experiment was obtained. The validity of force-force correlation functions in electron transport was investigated. We also considered scattering and screening effects in ultrasonic attenuation.

The driving force for thermomigration was examined. A linear-response expression was derived for the electronic component of the driving force. We calculated this force within Green's function theory.

RESEARCH OBJECTIVES

The object of this research was to investigate theoretically the driving force for electromigration and thermomigration in metals.

The driving force for electromigration was explicitly shown to be equal to the local electric field accompanying electron transport. The local field was evaluated using a density-matrix formulation and using the Green's function diagrammatic technique. Corrections to previous force expressions were shown to arise from scattering interferences, vertex corrections, and a local polarization effect contained in the off-energy-shell T-matrix. These contributions have been shown to be considerably smaller than the electron-wind contribution in simple metals when the mean-free-path is substantially larger than the electron wavelength at the Fermi energy. Bound states and virtual-bound states were included in the analysis for the first time in any published work. As a virtual-bound state is lowered in the conduction band its contribution to the force continuously approaches that of a true bound state. This would effectively modify the observed electrostatic bare-valence of some impurities, e.g., hydrogen, in metals.

Since the electron wind force is dominant in simple metals and can be most easily calculated using pseudopotential theory, we performed further calculations based on our earlier work. We considered the most realistic atomic configurations to date, incorporating lattice distortion and other structural arrangements never before considered. Lattice distortion effects typically can give 10%-30% corrections to the force. Calculations for the atomic configuration of a fast-diffuser complex show that the structural effects are appreciable and afford a possible explanation of observed anomalous behavior in these systems. Within the pseudopotential picture for nearly-free-electron metals, the structural effects associated with a grain

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boundary have little influence on the driving force for electromigration. Finally, our calculations show how configurational effects may account for the observed isotope effects in liquid metals (Häffner effect) and for an isotope-dependent force in hydrogen electromigration.

Electron-impurity scattering potentials, which would be of use in electromigration calculations, were investigated in terms of the effects they cause in electronic structure. Phase shift parameterization schemes were used and applied to studying the effect of alloying on electronic structure. Effects of lattice distortion were considered. Agreement between theory and experiment was obtained.

Electron transport was investigated within the framework of the Boltzmann equation and within linear response theory. The validity of "memory function" and force-force correlation function techniques was examined. The role of electron-impurity scattering and electron screening effects in ultrasonic attenuation was also considered.

We critically examined the driving force for thermomigration. The phonon-scattering effects require a non-adiabatic analysis. The electron-scattering effects were described by a linear-response expression similar in structure to that used for electromigration. We calculated the force using Green's function theory and obtained results similar to those obtained previously using semi-classical theory.

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PUBLICATIONS

1. Apparent Screening Breakdown Mechanism in Ultrasonic Attenuation, R.S. Sorbello, Journal of Low Temperature Physics 77, 141 (1976).

2. Effect of Alloying on the Fermi Surface, R.S. Sorbello, Physical Review B 15, 3045 (1977).

3. Local Fields in Electron Transport: Application to Electromigration, R.S. Sorbello and B. Dasgupta, Physical Review B 16, 5193 (1977).

4. Basic Concepts of Electro- and Thermomigration; Driving Forces, R.S. Sorbello, Electro- and Thermo-transport in Metals and Alloys, edited by R.E. Hummel and H.B. Huntington (The Metallurgical Society of AIME, New York, 1977), Chapter 1.

5. Electromigration in Liquid Metal Alloys, R.S. Sorbello, Physica Status Solidi (b) 86, 671 (1978).

6. Effect of Impurities on Electronic Structure, R.S. Sorbello, Journal of Nuclear Materials 69, 652 (1978).

7. Microscopic Fields and Currents in d.c. Electrical Conductivity, R.S. Sorbello, Electrical Transport and Optical Properties of Inhomogeneous Media, edited by J.C. Garland and D.B. Tanner (American Institute of Physics, New York, 1978), p. 355.

8. Strong Coupling Theory for the Driving Force in Electromigration, P.R. Rimbey and R.S. Sorbello, Physical Review B, accepted for publication.

9. Force on an Atom in an Electrostatic Field: Feynman-Hellmann Theorem and Oscillator Strengths, R.S. Sorbello and B.B. Dasgupta, Physical Review B, accepted for publication.

10. Electromigration in a Quasi-Two-Dimensional Electron Gas: Theory of the Driving Force, B.B. Dasgupta and R.S. Sorbello, submitted to Physical Review B.

11. Boltzmann Equation and Force-Force Correlation Function for Electrical Conductivity, R.S. Sorbello, submitted to Physical Review B.

12. Effect of Lattice Distortion on Electron-Impurity Scattering: Phase Shifts in the Distorted-Wave Born Approximation, R.S. Sorbello, submitted to Physica Status Solidi.

13. Atomic Configuration Effects in Electromigration, R.S. Sorbello, submitted to Journal of Physics and Chemistry of Solids.

14. Linear Response Theory of Thermomigration in an Electron Gas, P.R. Rimbey and R.S. Sorbello, submitted to Physical Review.

TECHNICAL PERSONNEL

In addition to the principal investigator the following technical personnel have worked on this grant.

Dr. Basab B. Dasgupta	(Postdoctoral Research Associate) - Theoretician. Worked on Liouville-equation approach to fields and forces in electromigration, dielectric response of electron gas, and electromigration in a quasi-two-dimensional electron gas.
Dr. Peter R. Rimbey	(Postdoctoral Research Associate) - Theoretician. Worked on Green's function theory of electromigration and thermomigration, with emphasis on many-body aspects of strong-coupling theory.

COUPLING

1. The Metallurgical Society of AIME, Fall Meeting 1976

   a. Richard S. Sorbello

   b. Conference (20-23 September 1976, Niagara Falls, New York).

   c. Presented invited paper "Basic Concepts in Electro- and Thermomigration: Driving Forces."

      Also had discussions with R.E. Hummel (University of Florida), P.S. Ho (IBM), H.B. Huntington (RPI), T. Hehenkamp (University of Gottingen), D. Rigney (Ohio State University) and D. Peterson (Ames Laboratory).

2. International Conference on Properties of Atomic Defects in Metals

   a. Richard S. Sorbello

   b. Conference (18-22 October 1976, Argonne National Laboratories, Argonne, Illinois).

   c. Present paper "Effect of Impurities on Electronic Structure."

      Also had discussions with C.P. Flynn (University of Illinois), A.M. Stoneham (AERE, Harwell), P.S. Ho (IBM), and R. Benedek (Argonne).

3. APS March Meeting 1977

   a. Richard S. Sorbello

   b. Conference (21-24 March 1976, San Diego).

   c. Presented paper "Local Fields in Electron Transport."

      Also had discussions with R. Landauer (IBM), H.B. Huntington (RPI), W.L. Schaich (Indiana University), L.J. Sham (University of California, San Diego), and P. Kumar (USC).

4. APS Topical Conference on Electron Transport and Optical Properties of Inhomogeneous Media

   a. Richard S. Sorbello

   b. Conference (7-9 September 1977, Columbus, Ohio).

   c. Presented paper "Microscopic Fields and Currents in d.c. Electrical Conductivity."

      Also had discussions with D. Stroud (Ohio State University), R. Landauer (IBM), A.B. Pippard (Cambridge University), and P.L. Taylor (Case Western Reserve).

5. Midwest Solid State Theory Conference

   a. Richard S. Sorbello

   b. Conference (21-22 October 1977, Argonne National Laboratories, Argonne, Illinois).

   c. Attended sessions and had discussions on electromigration and electron-impurity interaction with W.L. Schaich (Indiana University), P. Vashista (Argonne) and R. Benedek (Argonne).

6. Iowa State University Materials Science Colloquium

   a. Richard S. Sorbello

   b. Colloquium (4 November 1977, Ames, Iowa).

   c. Present review paper to Materials Science Department of Ames Laboratory. Had discussions on electromigration with electromigration experimental group including D.T. Peterson, O.N. Carlson, J.D. Verhoeven and F.A. Schmidt.

7. APS March Meeting 1978

   a. Richard S. Sorbello

   b. Conference (21-24 March 1978, Washington).

   c. Attended sessions and discussed theory of electromigration and electron transport with R. Landauer (IBM), H.B. Huntington (RPI), W.L. Schaich (Indiana University), P. Kumar (U.S.C.), F.M. Mueller (University of Niemegen), and W.E. Lawrence (Dartmouth).

8. Midwest Solid State Physics Conference

   a. Richard S. Sorbello

   b. Conference (6-7 October 1978, Argonne National Laboratories, Argonne, Illinois).

   c. Attended sessions and discussed electromigration, lattice distortion, and electron transport with R. Benedek (Argonne), G. Mahan (Indiana University) and N.L. Peterson (Argonne).

9. APS March Meeting 1979

   a. Richard S. Sorbello

   b. Conference (21-24 March 1979, Chicago).

   c. Presented paper "Strong Coupling Theory of the Driving Force for Electromigration." Attended sessions and discussed theory of electromigration and electron transport with H.B. Huntington (RPI), W.L. Schaich, G. Mahan and J. Swihart (Indiana University). Discussed experimental possibilities of hydrogen electromigration in palladium with R. Griesson (Vrije Universiteit, Amsterdam).

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